

Scientific Realism and Chemistry

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[DRAFT – please do not cite or circulate]

Introduction

Scientific realism is a philosophical issue with relevance to all sciences, but there are some particularly interesting and distinctive ways in which it has manifested itself in chemistry. Paying proper attention to such aspects and instances will deliver two types of benefits: first, it will aid the philosophical understanding of the nature of chemical knowledge; second, it will throw some fresh light on the realism debate in places where it has developed without much attention to chemical examples. In the following discussion, I will attempt to make a reasonably comprehensive survey of relevant literature, while also advancing some original points and viewpoints.

(1) *Unobservable entities*

Recall Bas van Fraassen's now-classic formulation of the realism debate as an argument about whether we can know about unobservable entities featuring in scientific theories (**quote**; van Fraassen 1980, **page**). If this is how we understand realism, in the long view of the history of science chemistry is the most important science to consider in the realism debate. Until the development of atomic, nuclear and elementary-particle physics starting in the early 20th century, chemistry was the science in which debates about the reality of unobservable theoretical entities took place with most ferocity and most relevance to practice. In astronomy there was a significant phase of the realism debate around the Copernican Revolution, but the conclusion of that revolution brought in a long and secure phase of realism about astronomical objects far out of reach of any human senses (including those that do not even register as tiny specks of light to our eyes). This underlying astronomical realism is unwittingly

reflected in van Fraassen's argument that the moons of Jupiter are observable entities because if we went near enough to them we would be able to perceive them with out unaided senses [page REF]. In contrast, the achievements of the early modern period only deepened the sense of inaccessibility and unobservability concerning the putative fundamental entities postulated in chemical theories.

Unobservability in chemical theories is not only an issue about atomism, though surely the problem was clearly present with the atomistic particles imagined by a wide range of thinkers from Democritus and Leucippus of ancient times to Descartes and other early-modern mechanical philosophers. More important for early chemistry than atomism were theoretical speculations about elements, conceived without much regard to the question of their atomistic constitution. For example, in the Paracelsian *tria prima* theory, the elements "sulphur", "mercury" and "salt" do not refer to the normal substances called by those names, which are perfectly observable [some convenient ref. on this]. Mercury, for example, was a theoretical substance embodying perfect fluidity and volatility, only imperfectly manifested in liquids such as mercury as we know it in everyday life; alchemists sometimes spoke of "the philosophical mercury" or "our mercury" in order not to be mistaken as meaning ordinary mercury. Hardly anyone imagined that the philosophical mercury could be directly observed.

The situation was similar with other fundamental substances of early chemistry, such as phlogiston; except for a very brief period when Henry Cavendish thought that inflammable air (hydrogen) was pure phlogiston, even chemists working in the phlogiston tradition did not imagine that phlogiston could ever be isolated in observable form. The situation was very similar with heat and electricity, both of which were standard chemical subjects in those crucial decades around the year 1800. Both were considered material substances capable of chemical combinations — electricity as one kind of fluid or two depending on one's theoretical allegiance, and heat as "caloric" (appearing at the top of Antoine-Laurent Lavoisier's table of chemical elements, along with light) [ref.]. Both were regarded as unobservable in themselves, though their effects were surely observable. Even something as straightforward-sounding as

Lavoisier's oxygen falls into the realm of the unobservable. In Lavoisier's own terminology, the substance he was handling daily was *oxygen gas*, which was a chemical compound made up of *oxygen base* and caloric [**primary and secondary ref.**]. Only the removal of all caloric present would have given the pure form of oxygen base, and no one expected such absolute privation of heat to be possible. So oxygen (base) was an unobservable entity, in quite a robust sense.

The question of unobservability only deepened with the advent of chemical atomism, most famously spearheaded by John Dalton and Jöns Jakob Berzelius at the start of the 19th century [**ref. Nye, ch. 1; Gardner**]. It is not that atomic ideas were absent in chemistry and physics earlier, but the question about their nature became urgent with Dalton and Berzelius probably because only they had succeeded to make atomism useful in chemistry [**ref. Chalmers**]. This situation needs a more careful analysis than is usually given. We need to start with a caution regarding the importance of the realism debate: even in the age of atomic chemistry, whether atoms "really existed" was mostly not a real concern to most working chemists, for about a century following Dalton's first publication on atoms in 1808 [**ref.**]. Alan Rocke makes a very useful distinction between chemical atomism and physical atomism [**quote and cite**]. He argues, and most knowledgeable historians of chemistry would agree, that chemical atomism was accepted by most 19th-century chemists but physical atomism was not so universally accepted, and moreover not necessary for most of the work chemists were doing.

It is easily imagined that chemical atomists, in contrast to physical atomists, were instrumentalists or even positivists, but that would be too simple. Chemical atomism, like any other theory postulating unobservable entities, could be taken in either realist or anti-realist way. Chemists were not always explicit about such issues, but I think many working chemists in the 19th century did believe that there was *something* real "out there" that constituted basic units of chemical combination and re-combination, possessing definite weights, though it was unknown what other properties they possessed. That is a different attitude from the positivism of saying that there were simply the stoichiometric regularities concerning how much of which substance combined with how much

of which other substances (expressed as “equivalents”), or the instrumentalism or fictionalism of saying that chemical combinations happen *as if* there were chemical atoms. Especially as structural organic chemistry developed in the middle decades of the century, I believe that most working chemists did begin to take chemical atoms as real entities. A crucial moment in this shift was the achievement of consensus on atomic weights and molecular formulas through the efforts of Stanislao Cannizzaro and others (at the emblematic Karlsruhe Congress of 1860, for example), and slightly earlier, through what Rocke calls the “quiet revolution” of the 1850s in organic chemistry [**ref. to Rocke, and Chang 2012, ch. 3**]. Confidence in the reality of chemical atoms, whose defining property was weight, understandably went up when various chemists could agree on what their weights were.

What else was considered real about atoms? This is a long and complex story. Dalton had originally assigned definite shapes (spherical) and sizes to atoms, and attempted to use them in various physico-chemical explanations of phenomena. Within his own theory he did not reach convincing determinations of these properties [**ref. to Fox**], and almost no other chemists took them seriously. Similarly, it was not till the advent of stereochemistry (chemistry in three-dimensional space) in the late 19th century that theoretical notions about *molecular* shapes were given realist credence by a large number of chemists, even though there was always a significant impulse towards realism concerning molecular shapes arising from crystallography [**ref. or further explanation**]. But even with the development and acceptance of stereochemical theories, the shapes, sizes and other physical properties of individual atoms remained beyond the reach of empirical determination until a whole new era arrived in physics. Similarly, even though structural chemistry gave clear indications of how many bonds each atom could and did form with other atoms, and even with what spatial orientation, the specifics of the mechanism of the chemical bond (represented with the deceptive simplicity of a line) remained obscure [**cross-ref. to later discussion**].

What philosophical sense can we make of the practices of structural chemists in the second half of the 19th century? Their science was wildly successful, in all kinds of ways, including the persuasive elucidation of the

constitution of a very wide range of substances and the facilitation of the synthesis of complex materials. The first thing to recall is that all of this achievement was made on the basis of a very partial knowledge of the physical properties and structures of atoms. And the 19th-century chemists were perhaps wise not to attempt to figure out such things with the material and conceptual resources available within their science. When the discovery of electrons and subsequently the development of quantum mechanics shed further light on the structure of atoms and the nature of the chemical bond, the picture that emerged was not like anything that 19th-century chemists imagined, or could have imagined.

What do these reflections tell us about the realism debate? The first point is that realism is not an all-or-nothing matter. One can be committed to the reality of some of the presumed properties of a theoretical entity, without a commitment to the rest. It is also possible (and perhaps necessary) that a theory itself only comments on some aspects of the entities in its domain and keeps silent about the rest. A theory can be highly successful on such a partial description of reality, and scientists can make successful use of a theory while making a realist commitment only to part of what it says about the unobservable reality. Either is an interesting indication that the success of a science (or some particular system of practice within it) is only an argument for the truth of some part of the theory. **[cross-ref. to further discussion of this point below] [ref. to existing discussions of “partial realism”, e.g. Dean Peters PhD, LSE 2012]**

And the question still remains whether all the successes couldn't have been achieved without *any* realist commitment **[quotations pro and con]**. But at least with an eye to typical human psychology and pragmatic constraints, I think the more plausible interpretation is along the lines of “operational realism” advanced by Bernadette Bensaude-Vincent and Jonathan Simon **[ref; and discuss my own emphasis on operationalization]**. This is the kind of cautious commitment that has been characteristic of modern chemists, steering a middle course between realist enthusiasm and anti-realist skepticism **[and it can apply to both entities and properties]**.

(2) *The nature of models*

In philosophy of science recently there has been a recognition that much theoretical work in science happens by means of models, rather than anything billed as “theories” or “laws”. This is very much based on how scientists themselves speak about their practice these days. In chemistry, compared to the kind of physics that informed traditional philosophy of science, there is a much longer history of a conscious use of models, and chemists have often debated the epistemic function of models and the ontological status of the entities postulated in the models. This is quite interesting from the viewpoint of the realism debate. To call something a “model” has significant anti-realist connotations — a good “theory” can be imagined to fit reality perfectly, but a “model” would seem like something we have to make in lieu of a full and accurate theory, or something that intentionally incorporates simplifications for practical purposes. Yet, there is also realist intent in modelling in many cases, a desire to make a partial or approximate representation of reality, faithful within its acknowledged limits. This is consonant with the view expressed **in Section 1** that successful scientific work can be, and often is, carried out on the basis of a partial realist commitment to a theory concerning unobservables.

Such partial realism (of varying degrees) is exemplified very well in the history of models in chemistry since the early 19th century. Chemists’ attitudes towards their models have been various and changeable, but rarely have they been fully realist or fully anti-realist. Some models, such as the stacking of unit cells in crystallography, were always taken quite literally, but even there the realist commitment was partial for most of the history, in the sense that the models only concerned the (presumably undeformable) spatial shapes of the cells and not any other properties that the cells might possess. As Christoph Meinel has shown in illuminating detail [[ref.](#)], the structural models of organic chemistry began mostly as heuristic and pedagogical tools and only gradually acquired higher realist significance. The most famous type was the “ball-and-stick” models originating in the 1860s with August Hofmann’s rigging-up of croquet balls connected with sticks drilled into them, with which he expressed the notion of valency (valence) that he was helping to articulate. Hofmann’s

models are the direct ancestors of the colorful ball-and-stick sets that continue to aid the thinking of chemists, chemistry students and the public to this day.

The ball-and-stick models are taken quite literally today, as far as the spatial arrangements of atoms are concerned (despite the quantum-mechanical qualms one would generally have about such a classical representation). However, this was not always so, even when the models were quite successful for their purposes. Hofmann himself clearly lacked full realist ambitions for his models, as he kept them 2-dimensional, and he made no attempts to theorize about bond lengths (and therefore exact molecular shapes), keeping all the sticks the same length [**details/evidence from Meinel**]. The nature of the epistemic move involved in making and using such models become clearer when we consider representations that were definitely not meant to be taken literally [**or what is the graphic equivalent of “literally”?**]. For example, consider August Kekulé’s “sausage” models in which atoms were represented as sausages of different lengths, the length indicating the valency of each atom; it was certainly not Kekulé’s intention to argue that atoms really were sausage-shaped. There is also the earlier case of Auguste Laurent’s “prism” model [**details**], which was not intended in a realist way even though it was actually a 3-dimensional model [**refs on K. and L.; Freund on the latter?**].

There have also been important chemical models that were not spatial at all, and in that sense not even trying to be realistic depictions of atoms and molecules. For example, what exactly was the epistemic status of chemical formulas, famously designated as “paper tools” by Ursula Klein [**ref.**]? There were many ways of dissecting the compositional formula of a molecule into its presumed component parts. [**an illustrative example; the 18 ways of understanding ether?**] There were various ways of convincing oneself that some presumed parts were real [**cross-ref.**], but Klein’s point is somewhat different: the manipulation of the formulas themselves was a distinct method of chemical reasoning and research, and the formula for each presumed grouping of atoms was a model-element, a conceptual tool with the help of which various theoretical aims were achieved. Did success in such theoretical work confer reality to what those formulas represented? For example, should various Berzelian radicals have been considered real because they facilitated some

important explanations and predictions of various chemical reactions? [**ref. to Ihde for convenient summary**] Or should one have reserved reality for only those elements that were manifested in a more direct way in experimental settings, for example as products of electrolysis [**cross-ref. to section 3**]? There was no consensus among chemists on this issue, and it is difficult to see that there is a clear answer that they should have agreed on.

It is interesting to observe how chemists have sometimes changed their attitudes toward certain models, and to discern what it is that they felt warranted such a transition. For example, the concept of valency began as an abstract notion of combining power expressed with the help of heuristic graphic models (such as Kekulé's sausage formulas and Hofmann's sticks coming out of balls). Even though the combining power itself would have been considered real by many chemists, there was little indication that the heuristic pictures should be taken as representations of reality. This all changed with the advent of stereochemistry [**ref. to Ramberg**], [**story about optical isomers**]. Tetrahedral carbon makes an interesting story. Those who took the quadrivalency of carbon seriously in a realist way could only conclude that the shape of the carbon atom had to be tetrahedral, if its bonds (four sticks coming out of the ball in Hofmann's models) were to be distributed symmetrically in 3-dimensional space [**the payoff of this symmetry assumption, e.g., concerning the absence of CH_2R_2 isomers**]. The success of tetrahedral carbon marked a clear transition in the ontological status of valency. But what *were* these bonds, if they were to be taken in a realist way as physical entities? No answers were possible within the tradition of 19th-century structural chemistry, which did not have any account of the internal structure of atoms. Through the 20th century the phrase "atomic structure" has become very familiar, but it would have had a clear oxymoronic ring in the 19th century, when "atom" still meant an indivisible unit, therefore lacking any meaningful internal structure by definition. [**what does that show?**]

Debates about the reality of various models in chemistry did not cease in the 20th century. When Gilbert Newton Lewis began to make his creative use of the newly discovered electron in his theorizing about chemical bonds, starting with his model of the cube that was completed by 8 electrons, it was not clear that this alleged distribution of electrons in the space around the atomic nucleus

should be taken seriously in a realist way. The same kind of question arose with other schemes that tried to use the distribution of electrons to explain the periodicity of chemical elements, including J. J. Thomson's and Niels Bohr's [**ref. to Arabatzis ch. 7**]. None of these models were based on any credible physics of how an electron moved and interacted with a nucleus and other electrons, so it was perhaps easy enough to be anti-realist about them. However, the existence of a worked-out theory behind a model is not necessary for that model to be taken in a realist way; consider the early realist Copernicans, who had no credible theory of kinematics or dynamics about how the earth could be spinning with no apparent sign of that motion. Even though the Lewis cube did not survive the test of time and further work, a related idea from him did: electron-pairs. Lewis had no theoretical basis, except a magnetic analogy, for believing that electrons should or even could form stable pairs in the way that his scheme of chemical explanations demanded. It is extraordinary that later developments in theoretical physics provided justification for electron-pairs in a manner that Lewis could not have anticipated, through the concept of spin and the Pauli exclusion principle. [**and Lewis himself did not like quantum mechanics, when it came!**]

The advent of full-fledged quantum mechanics and its application in chemistry did not stop the use of models and modelling techniques of debatable realist credentials. The most obvious case is that of orbitals, which have assumed a curiously strong realist presence in the mind of many chemists and chemistry students. Strictly speaking, orbitals are just mathematical functions. In the simplest form they are the eigenstates of the Hamiltonian (energy) operator in a one-electron atom. [**ref. to existing discussions on orbitals, including Scerri's reaction against their presumed direct observation**] In so many textbooks these functions are reified in nice graphic representations, and the explanations of the periodic table typically imagine electrons coming in to occupy different orbitals in a specific order, as if the orbitals were so many pigeonholes waiting for different pigeons to occupy them. In the context of the realism debate, it is difficult to know what to make of the great success of orbital-based chemical reasoning. There would seem to be no good reason why orbital models of multi-electron atoms should work so well. Electrons within a given

atom are strongly interacting with each other, so the orbitals derived from the solution of a one-electron Schrödinger equation are at best crude approximations for orbitals in a multi-electron atom [**comment here on how MO deals with this? or say how this is a different concern**]. Electrons are also truly indistinguishable from each other if we take quantum mechanics seriously, so the talk of different electrons occupying different orbitals within the same atom does not make sense. And why should we believe that electrons in an atom exist in eigenstates of the Hamiltonian, rather than in a superposition of various eigenstates? So what sense is there in thinking that a given electron is always in one orbital or another? Given all these difficulties with taking the pigeonhole picture of orbitals literally, should we conclude that the success of orbital-based reasoning is just one great lucky coincidence? [**cf. Scerri's "miracle" comment**, though it's not really quantum mechanics as physicists know it that explain the periodic table, as Scerri himself points out] If we don't want to do that, then we have a challenging task: to spell out exactly in which ways the orbital models get reality correctly in such a way as to underpin extremely effective explanations and predictions. [**This exemplifies a fundamental difficulty of partial realism – more on this later.**]

[**Similar questions can be, and has been, raised about Linus Pauling's resonance concept. Discuss w/ ref. to Gavroglu and Simoes.**] [Also Coulson's anti-realism about the chemical bond. **Discuss w/ ref. to Hendry**] [**Grant: what can I say briefly about "curly arrows" here?** And your point about the incommensurability of competing representations where you refer to Lopes? Has that been published?]

(3) Interventions and practical success

Is there a way to move beyond the underdetermined situation as just discussed, in which we know that a theory or model is successful but pinpoint which aspects of it deserves realist credence? In that context it is easy to see the appeal of Ian Hacking's doctrine of "experimental realism", that reality can be ascertained by successful intervention [**quote and cite**]. Experimental realism has an initial resonance in chemistry, even though Hacking's own inspiration came from other fields of science such as modern experimental high-energy

physics and biological microscopy [refs.]. [the epistemological importance of practical interventions – **“If you can spray them, they’re real.”**] It is commonly acknowledged that chemistry has always been a laboratory science with close ties to technology and industry, a distinctly “impure science” as Bensaude-Vincent and Simon put it. Chemical knowledge has always been founded on the practical manipulation of substances, and chemists have been proud of their ability to make things [**Berthelot’s comment**: “chemistry creates its objects”]. Modern synthetic chemistry is perhaps unique among the sciences (at least until synthetic biology develops further) in its ability to create a dizzying array of well-specified entities, many of which are not even known to form spontaneously in nature. Who would dispute the reality of these substances that chemists create by careful design, which they can also use as tools for achieving certain desired effects so well? So it may seem that chemistry, the science of intervention *par excellence*, should give the best instantiation of Hacking-type experimental realism. While that impression has a strong element of truth to it, further consideration reveals some difficulties that in fact point to an important weakness in experimental realism.¹

Let me come to the difficulties first, and then return to the more positive view to see what can still be retained in the spirit of experimental realism. The basic critical point is that in chemistry Hacking’s idea is especially prone to attack from the pessimistic (meta-)induction from the history of science [**ref. Laudan; Psillos**]. All sorts of entities such as phlogiston and caloric have been used as bases for successful chemical practices, so it becomes difficult to deny their reality on experimental-realist grounds. Chemistry is full of examples of successful theoretical schemes containing entities that we now take not to exist and assumptions that we now take to be false. For example, Joseph Priestley

¹ It is useful to distinguish two strands of the realism debate, concerning existence (or reality) and truth: (1) do the unobservable entities postulated in our theories really exist (and do we know that they do)? (2) are the statements concerning unobservables made by our theories true (and do we know that they are)? The second strand does include the first if we consider the statements made by theories to include existential statements concerning unobservables, but the two are often treated separately. That is Hacking’s own inclination when he bills his own position as “entity realism” [ref.]. [**But even in entity realism it’s not just bare existence that we presumably know about; basic causal properties are involved.**] [also note **Woodward connection**]

predicted, on the basis of the phlogiston theory, that a metallic calx (oxide) combining with inflammable air (hydrogen) would be reduced to pure metal, because calx is de-phlogisticated metal and inflammable air is full of phlogiston. This prediction was brilliantly confirmed in an experiment in which he used a large “burning lens” to focus sunlight on lead calx enclosed in inflammable air [ref. to Musgrave, and my own more extensive discussion; and Priestley’s original paper]. Isn’t this just the kind of intervention that Hacking has in mind as the basis of his experimental realism? Wasn’t Priestley “spraying” phlogiston on to the calx, using phlogiston successfully as a tool in order to achieve a very distinct and practical experimental intervention? If so, there would seem to be no reason to decline to regard phlogiston as real. **[and add the phlogiston-as-electron story here]**

This is not only about the bygone ages of chemistry with no relevance to modern chemistry. Some of the examples discussed above in **Section 2** are very instructive. The spectacular practical success of organic structural chemistry in the 19th century owed much to models that were not regarded as literally true even at the time. The situation does not change if we come into the age of quantum chemistry from the 1930s onward. Not only a great deal of theoretical reasoning but numerous experimental interventions rely on the concept of orbitals and on detailed knowledge about the number and shapes of various types of orbitals, while orbitals have no reality if we take quantum mechanics literally. What these examples illustrate is that experimental success is no guarantee of the reality of the entities that the experimenters *presume* to be manipulating when they carry out their experiments. To carry on with Hacking’s slogan: you may be able to spray something without knowing much about what it is that you’re spraying. All you can perhaps be sure about is that there is some “it” that you are spraying, but Hacking’s slogan doesn’t work as intended if the blank “it” (or “them”) is filled in with something concrete: “If you can spray phlogiston, then phlogiston is real.”

But why do I say that chemistry is particularly prone to the pessimistic induction, rather than just as prone to it as any other science is? Paradoxically, this is because of the very practical nature of chemistry: at least in modern chemistry, it is not a likely occurrence that a theoretical idea becomes widely

accepted without having proven itself by supporting some measure of practical intervention. This has been the case at least since the advent of affinity-based chemistry in the 18th century. Yet, as in all sciences, ideas and theories do change, sometimes radically, in chemistry. Then it must be quite easy to find chemical theories that are now rejected (or at least considered false) but has quite a firm grounding in practical interventions. Or at least such theories must have supported some interventions successfully, and that practical grounding must still be present unless nature itself has changed in the meantime.

If my argument is successful, perhaps it will make people turn away from Hacking's experimental realism; my intention, however, is just the opposite. Rather than despairing about Hacking's experimental realism because it would rule phlogiston in, I want to suggest that we should continue to appreciate the strength in Hacking's position and learn to accept that phlogiston *is* real — or at least as real as any other unobservable theoretical entity. The attitude I am promoting here is linked to what I have called the "optimistic rendition of the pessimistic induction" [**explain, and ref.**]. This is part of what I call "active realism", which is the commitment to learn from reality in all possible ways; each concept facilitating successful interventions provides ways of learning from reality, and should be maintained and developed as much as possible.

Seen from the perspective of active realism, the history of chemistry is an exemplary source of object-lessons in Hacking's experimental realism, as well as Bensaude-Vincent's operational realism [**refer back, or just do here**]. There are many other important examples. From early chemistry, we have the widely accepted norm that the constitution of a chemical substance ought to be confirmed by its decomposition into its presumed components, or by its synthesis from the components. The neatest demonstration of composition was given by a combination of successful decomposition and recombination. This ideal was exhibited in a whole range of successful chemical work, including Georg Stahl's early work on sulphur and metals (which Kant admired so much – **ref.**), Lavoisier's work on the composition of water, Berzelius's electrochemical theory grounded in results of electrolysis, right down to the triumphs of industrial chemistry starting in the late 19th century. Slightly different but closely related was the work on substitution: chemists gained a great deal of

constitutional knowledge, starting from the mid-19th century, by the technique of substituting one part of a molecule with another atom or radical. This began with the rather accidental discovery of hydrogen–chlorine substitution in organic chemistry, a reaction deemed rather incredible from the framework of Berzelian dualistic theory, as hydrogen was highly positive and chlorine highly negative. Substitution played a key role in generating realist confidence in molecular structures, and in helping chemists arrive at the concept of valency, which was of enormous benefit to the progress of chemistry and still remains essential in much of chemical reasoning. [ref. Chang 2012, ch. 3 on the substitution-type system]

(4) Preservative realism vs. conservationist pluralism

I have made several indications above that theories providing the underpinnings for successful investigations deserve our realist confidence, and that such theories (or some elements or aspects of such theories) tend to be preserved through the ages. All this may sound suspiciously like the position that I have critiqued as “preservative realism” [Chang 2003]. Therefore it is necessary for me to distinguish my own view carefully from that position, and articulate more clearly what I think about when, why, and how successful theories are and should be preserved.

My basic critique of preservative realism remains: a mere preservation is not an argument for truth, not even for the modest quotidian sense of truth (meaning reasonable confirmation by tests that we can perform). We need to consider what kinds of things tend to get preserved through major theoretical changes, and see whether those things can support realism. The survival of a good amount of old data would seem to be a fairly typical feature of scientific change, despite the highly publicized extreme cases in which the data themselves did change. Similarly for phenomenological laws, which represent the data in a convenient mathematical relationship without relying on causes, mechanisms, and far-reaching theoretical principles. The preservation of phenomenological laws would seem to be a general feature of scientific development, as stated by various philosophers ranging from Herbert Feigl to Nancy Cartwright [refs.]. But the preservation of experimental data and phenomenological laws, all of

which lie in the realm of the observable, will not give the realists what they want; nor will it trouble any empiricist anti-realists.

We also often witness the preservation of aspects of scientific theories that are determined by our own habits of thinking rather than by nature, and these are also no help to the realists. First, there are techniques of representation and reasoning, including certain mathematical methods, that we just find convenient to use. Linearity would be a good example. And then there are deep-seated metaphysical commitments. A good example here is the desire for a conservation principle, which have led scientists to anchor their theories on various conservation principles (concerning mass, *vis viva*, heat, energy). Most of these principles were empirically refuted and rejected, but that has not stopped scientists from simply moving on to some other conservation principle; we still have energy conservation, but we also know that it is not so simply and precisely obeyed in the realm of quantum field theory. Such metaphysical propositions or inclinations, which also include determinism and atomism (and their antitheses, **ref. Holton on themata**) “can be held true come what may”, to borrow Quine’s phrasing that was meant to apply more broadly. The fact that certain of these metaphysical beliefs have been preserved by most European scientists for the past few centuries is, in itself, no indication of the way the world is or of what we know about it.

The preceding discussion should also serve as a reminder of the fundamental difficulty with partial realism [**cross-ref. to earlier discussion**]: it is difficult to tell which parts of a successful theory are responsible for its successes. Copernicus might have attributed his success to his obstinate and purist preference for uniform circular motions that crucially helped him to reject Ptolemaic astronomy [**ref. Kuhn**]. In the realm of chemistry, should we say that Lavoisier’s success was due to his theory of caloric, which allowed him to believe that he had reached a satisfactory explanation of the heat issuing in combustion, freeing him to discard the phlogiston theory and focus on oxygen and weight-based explanations and investigations? Discerning the real secret of success is bound to be difficult for those mixed up in the creative process while it is in progress. But even with the luxury of “20-20 hindsight” it is not easy to tell what was truly responsible for the success of a theory; an illustration of that difficulty

is the fact that intelligent and well-informed people (such as Stathis Psillos and myself!) had to argue it out in print on such a mundane case as the caloric theory of heat [ref. Chang; Psillos].

The only strategy we can employ in dealing with this difficulty is the same kind of detective work that happens in any scientific investigation, and in combatting the problem of underdetermination in theory-confirmation (scientifically and philosophically), rather than anything peculiar to the realism debate. And as this is not the kind of situation in which we can do systematic large-scale trials, we may be reduced to the kind of homely reasoning exemplified in John Stuart Mill's inductive methods of reasoning [ref.]. The method of difference should figure largely in this. [**can we get the same result without this assumption? etc.**] Some of what we need to know here is provided by history, in the form of actual variations among past scientists; some we can try to reason out through counterfactual history; in some cases we may actually have to try doing without certain elements of theory ourselves, by making calculations or doing experiments.

By such methods we can and should distinguish the operative parts of a theory (the "working posits") from the idle parts (the "presuppositional posits") [ref. Kitcher, etc.], but without any pretensions to ultra-mundane confidence. My caution here is threefold. First, what is operative in a theory will depend on which particular use we are making of it; for example, atomic sizes were operative for certain physical explanations Dalton attempted to make, but they were idle in most reasonings in the atomic chemistry of his time. Second, in each situation we may err in identifying what is operative and what is idle; here we can always challenge each other and correct ourselves, the way scientists do. But even supposing that we have made the best possible discrimination between operative and idle parts of a theory, we still have no guarantee that the operative parts are true in any eternal, universal and supra-operational sense; here enter all the familiar skeptical anti-realist arguments, ranging from the existence of empirically equivalent but mutually conflicting theories to Kyle Stanford's "problem of unconceived alternatives" [refs, van Fraassen for the former?].

Success is no guarantee of truth. Rather, I think success should be appreciated for what it is, and what seems to be responsible for success should

be preserved so that it may continue giving us that success. Now, when we say that a theory has been applied successfully, it is of course possible that it is actually some strange coincidence that led to the successful result. This is ultimately the fatal weakness of the argument for realism from the success of science, and I think the prudent thing is to accept that weakness for what it is. Yet, if our use of a theory has led to successful outcomes, and as far as we can check this is not the result of some coincidence, then we can and should say, modestly and provisionally, that the relevant statements made in this theory are true and the entities presupposed in them exist, in the same sense as we say that it is true that rabbits exist, they have whiskers, and they live in underground burrows. This “truth” is of the operational, verifiable kind, and is one and the same thing as empirical confirmation taken in a broad sense [**ref. to 5 senses of “truth” in Chang 2012**]. Here, again, it is important not to fall into delusions of grandeur.

From the “active realist” point of view, what success gives is merely a credible promise of more success, and we must accept this promise with eyes wide open to the problem of induction. When there is a theory that has time and again supported a successful operation, we say it applies well to that operation, and we have reasonable grounds for using it again for the same operation. If this theory in the same way supports a range of operations, those operations define a domain in which the theory is successful. When we have such a theory, we have reasonable reasons to expect that it will continue to be successful in the same domain, and that it may be successful in some adjacent domain, too. So it makes sense to keep that theory for future use. That is the only argument for preserving a successful theory; it is a modest and good argument. And such preservation, because it is firmly rooted in practical experience and the kind of basic induction that Hume taught us we can’t do without, should be robust in the face of another theory that does something else, or even the same thing, well. That is how we get conservationist pluralism [**quote from Chang 2012**].

[**Discuss Ladyman’s 2011 paper on phlogiston here**] [For me, structural realism only has force as a species of preservatism.] [Pauling should come in here – and why do structural realists ignore such an obvious and large case for them? But I suspect it’s not the kind of structure they want.]

(5) Reduction and levels of analysis

I cannot conclude this discussion of the realism debate concerning chemistry without discussing its relation to another important philosophical issue, namely reductionism, especially the variety of it referred to as “microreductionism” [**ref. to Chang forthcoming, and explain its relation to this paper**]. The epistemic or methodological project of (micro)reductionism begins with a belief in ontological (micro)reduction, because it is the latter that confers initial plausibility and promise to the former. So, if we believe that chemical substances are made up of molecules, which are in turn made up of atoms, which are in turn made up of elementary particles, it will be a very tempting thought that the best way to really understand chemical substances is to consult what elementary particle physics tells us about the nature and interaction of their component parts. That is to say, it is realism about the micro-level entities and their role as building-blocks of macro-level entities that generates a push for reductionism. It is because of their realist confidence in the reality of elementary particles and the truth of the theories given by physicists about them, that chemists are often inclined to accept the epistemic microreduction of their science to physics. Without that underlying realism, chemists would stay at the phenomenological level of investigation, or seek theoretical guidance elsewhere.

That much is simple enough. But as it often happens, putting a general idea into practice reveals many interesting subtleties and difficulties. In particular, we encounter a question about the right level of analysis, the answer to which remains open even if one accepts the reductionist ontology fully. The most productive level of analysis in quantum chemistry has turned out to be that of electrons and nuclei. But what ontological level is this? It is not one that any single theory of physics would recognize as a coherent domain. When quantum mechanics took shape as a full-fledged theory in the hands of Werner Heisenberg and Erwin Schrödinger, it turned out to apply very well to electrons in an atom but not to the atomic nucleus. Ordinary quantum mechanics, and its application in quantum chemistry, only use the nuclei as a source of a fixed electrostatic potential [**cross-ref to earlier discussion**], rather than providing answers about

their dynamics or internal structure [**qualify this statement**, in relation to how quantum chemists might handle nuclear motions in the next iteration]. The early models of atomic nuclei, such as the “liquid-drop” model or the shell model, had no comment at all to make about how the nuclei would interact with electrons, and in this respect even quantum chromodynamics is no better. One could take a more principled and generalized approach and start from the framework of the Standard Model, which encompasses all of the elementary particles including electrons, protons and neutrons. However, finding a “grand unified theory” governing all of these particles has been a challenging task it itself to say the least, and no one has made a credible attempt to set up a single equation or a single model to describe an atom or a molecule in that framework. As far as the current best practice goes, science treats the atom as a heterogenous composite made up of electrons and nuclei, much like what John Dupré says about how biology (rightly) treats a pig [**quote and cite**]. And this heterogeneous ontological picture is the basis of what has turned out to be a spectacularly successful system of chemical practice.

It would be fair to say that chemistry has always been committed to a reductionist ontology, with a degree of realism about the layer(s) of existence “underneath” the observable layer. But it is also clear that this general commitment to ontological reductionism and realism has not dictated very much about the exact direction of chemical practice. First of all, there is the axiological dimension of the realism question: is the fundamental aim of chemistry to seek correct descriptions of chemical phenomena in terms of the ultimate constituents of matter, or rather to seek the most effective description at any plausible level? On the whole, practicing chemists have tended to have the latter inclination, though that has by no means been universal. At least up to the mid-19th century, those who insisted on instrumental effectiveness tended to have the upper hand in chemistry, against the mechanical philosophers, metaphysical Newtonians, Boscovichians, Proutians, and others who prized the attainment of true microphysical descriptions above all. The great success of microphysics in the early 20th century changed this picture significantly, but the debate still continues: for example, many chemists would defend the continuing use of orbitals and electron shells for their instrumental usefulness, even though

fundamentalists declare them to be non-existent. In having this sort of internal disagreement the chemists are, of course, not unique: even within physics there are plenty of practitioners in areas such as solid state physics who decline to look entirely to elementary particle physics as a source of useful theoretical concepts and assumptions.

Summary

Chemistry, like any other science, is a realist enterprise in the sense that it seeks to learn from reality. But its practices are quite far from what standard realist philosophers might imagine. A close attention to chemical practice reveals **[a few more thoughts here]**.

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